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VARIATIONAL CALCULATION OF ELECTRON ELASTIC SCATTERING
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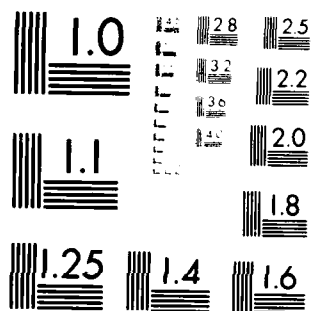
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VARIATIONAL CALCULATION OF ELECTRON
ELASTIC SCATTERING BY ATOMIC HELIUM

THESIS

AFIT/GEP/PH/82D-3 Paul J. Chernek
Lieutenant USAF

Approved for public release; distribution unlimited

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VARIATIONAL CALCULATION OF ELECTRON
ELASTIC SCATTERING BY ATOMIC HELIUM

Thesis

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University

In Partial Fulfillment of the Requirements for the
Degree of Master of Science

By

Paul J. Chernek
Lieutenant USAF

Graduate Engineering Physics

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Paul. J. Chernek

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Abstract

The elastic-scattering of electrons from atomic helium in the ground state is investigated. It is shown that for low energy incident electrons the scattering problem reduces to solving an ordinary integro-differential equation for the scattering wave-function. A method is discussed to obtain approximate solutions to the integro-differential equation by variational principles. The extremum condition of the variational method is formulated into a general $N \times N$ matrix equation which reduces to a 2×2 eigen-value matrix problem for the phase-shift of the scattering electron. An algorithm is presented to obtain the collisional cross-section for elastic scattering as a function of incident electron energy,

I. Introduction

Background

It is well-known that approximate methods based on variational principles are among the most powerful techniques used in solving quantum mechanical problems. In bound-state calculations, the Raleigh-Ritz variational method gives energy eigen-values which are correct to second order in the error of an assumed trial wave-function. The method also determines the free parameters of the wave-function and guarantees that the calculated eigen-values are upper bounds to the exact energy eigen-values of the bound system.

In scattering theory however, the total energy of the system is specified in advance. Variational principles are used to determine to first order the free parameters of the trial wave-function which contain all information of the scattering event. Unfortunately, no general bounding conditions are yet known on the solutions of the continuum problem calculated by variational methods. Thus there exists no defined standard (e.g., upper or lower bounds) with which to compare computed results using different trial wave-functions.

In spite of this difficulty, variational principles applied to scattering problems offer several advantages over other approximation methods. First, variational methods require, in general, far less numerical effort than non-variational methods. Second, results obtained by variational calculations, although not internally bounded, compare favorably with those obtained by more powerful non-variational techniques. Finally, physically complex interactions such as polarization and electron correlation effects can easily be included in a variational calculation within the assumed forms of the trial wave-functions. It is for these reasons that variational principles are still competitive with other more powerful non-variational scattering techniques.

The first serious attempt to apply variational principles to electron-helium scattering was made by Moiseiwitsch (Ref. 1).

Using the variational method proposed by Hulthen (Ref. 2) and a two parameter trial wave-function, Moiseiwitsch found good agreement (10%) for the S-wave elastic scattering phase shift with the known numerical solutions of the same integro-differential equations performed earlier by Morse and Allis (Ref. 3). Moiseiwitsch further suggested that improved results could be obtained by more complex trial wave-functions.

In a detailed study of variational principles applied to continuum problems, Schwartz (Ref. 4) first noted that at certain system energies variational calculations possess intrinsic anomalous behavior. He showed that as more complex trial wave-functions and more adjustable parameters are added to the variational calculations, the solutions do not converge uniformly, and can turn out totally erroneous for specific incident electron energies. Schwartz also studied the nature of these anomalies. He showed that although a trial set of functions is linear with respect to a set of corresponding parameters, the quantity which is extremized is the expectation value of the scattering Hamiltonian operator. This quantity is always quadratic in the parameters of the trial wave-function. As a result, the parameters of the wave-function have, in general, two roots, only one of which is physical. At certain system energies these roots can be complex and the variational method will break down.

Several attempts have been made to eliminate the anomalous nature of a single variational method by combinations of two different variational methods. Conditional calculations proceed in the same manner as a single variational method. However, when anomalous results begin to appear in one variational calculation, a transfer is made to a second variational method. Although two independent methods possess intrinsic energy anomalies, they do not, in general, occur in the same energy regions. Thus by alternating back and forth whenever a single method fails, accurate results have been obtained over the entire spectrum applicable to the physical limitations of

the approximations made.

Malik (Ref. 5) and Rudge (Ref. 6) proposed combining the variational method of Hulthen and Kohn (Ref. 7). Application of this technique has been only applied to electron-hydrogen scattering by Rudge (Ref. 6). Nesbet (Ref. 8) proposed the method of combining the variational principles of Kohn and the Inverse Kohn, Rubinow (Ref. 9). Both combinational methods demonstrated the anomaly-free nature of the technique but were restricted in practice to elastic scattering for hydrogen, since the methods could not be generalized to include inelastic scattering.

The most successful anomaly-free variational technique is the Transformation Method, Harris and Michels (Ref. 10). This method introduces a transformation which ensures that the anomalous energy regions are forced outside the range of the energy spectrum of interest. Application of the transformation technique to variational calculations of electron elastic scattering from helium was first performed by Michels, Harris and Scolsky (Ref. 11). This work was extended by Sinfailam and Nesbet (Ref. 12). Trial exponential wave-functions with decreasing numerical indices were used. The results of the calculations of the cross-sections compared extremely well (3% estimated probable error) to the experimental measurements of Golden and Bandel (Ref. 13).

Nesbet (Ref. 14) refined the calculations of Sinfailam and Nesbet (Ref. 12) for electron elastic scattering from helium. The results for the cross-section compared extremely well (1.5%) with the best non-variational technique, the R-matrix Method, O'Malley, Burke and Berrington (Ref. 15). The Nesbet (Ref. 14) calculation represents to date the best variational results on the electron-helium elastic scattering cross-section.

The single drawback of the anomaly-free variational methods is the increase in numerical labor required above the simpler variational calculations. Recently, Shankland (Ref. 16) proposed a variational

method which retains the simplicity of the single variational approach. Recognizing that a single variational method fails only in small energy regions near non-physical anomalous poles, he proposed a simple interpolating technique to obtain an accurate cross-section in the singular regions. If successful, this method will reduce the numerical labor required for computing accurate elastic electron-atomic cross-sections over a large energy spectrum.

Objective

In the present work, the Shankland Variational Method is formulated for the electron-helium elastic scattering problem. Specifically, an algorithm is developed to obtain variational solutions for the scattering phase-shifts as a function of incident electron energy.

Approach

In Chapter II the basic formulation of the electron-helium scattering problem is presented. In particular, the close-coupled formulation is discussed. Specifically, the simplest case of the closed-coupling method, the one-state approximation, is developed in detail. In Chapter III the Matrix-Variational Method is formulated. First the general variational method is applied to the electron-helium scattering equation. Second the results of the variational formulation are developed into a matrix eigen-value problem. In Chapter IV a detailed algorithm is presented for the calculation of the elastic scattering phase-shifts as a function of incident electron energy. Finally, an interpolation method is discussed for the special case in which the Matrix-Variational Method mathematically yields anomalous results. Appendix A is a compilation of the A-Matrix elements required in the computation. Appendix B is a compilation of the B-Matrix elements also required in the computation. Appendix C is a compilation of the definite integrals used throughout the calculation.

II. The Quantum Mechanical Problem

Basic Formulation

In this section the quantum mechanical formulation of electron impact with helium will be presented. The basic framework for this approach can be found in a number of articles, Massey (Ref. 17), Moiseiwitsch and Smith (Ref. 18), as well as texts by Mott and Massey (Ref. 19) and Geltmann (Ref. 20). In the following, the formulation presented by Mott and Massey (Ref. 19) is the most convenient. Atomic units will be used throughout, (Ref. 19).

The wave equation for the scattering of an electron by a helium atom is given as

$$\left(\nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \frac{4}{r_1} + \frac{4}{r_2} + \frac{4}{r_3} - \frac{2}{r_{12}} - \frac{2}{r_{13}} - \frac{2}{r_{23}} + E \right) \psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \vec{r}_3\sigma_3) = 0 \quad (2.1)$$

where r_1, r_2, r_3 are the distances of the three electrons from the helium nucleus, r_{12}, r_{13}, r_{23} are the distances between the electrons, and E is the total energy of the system. The total system wave-function $\psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \vec{r}_3\sigma_3)$ is an anti-symmetric function in the spin-space coordinates of each pair of electrons.

The standard method of attacking the general N-body scattering problem is to expand the total system wave-function in terms of the orthonormal set of target wave-functions. For electron-helium scattering we simply have

$$\psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \vec{r}_3\sigma_3) = \sum_{n=0}^{\infty} A_n \psi_n(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) F_n(\vec{r}_3\sigma_3) \quad (2.2)$$

where $\psi_n(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2)$ denotes the n^{th} state system wave-function for the unperturbed helium atom. It is an anti-symmetric wave-function in the spin-space coordinates of the helium electrons and is a solution to the helium equation

$$\left[\nabla_1^2 + \nabla_2^2 + \frac{4}{r_1} + \frac{4}{r_2} - \frac{2}{r_{12}} + E_n \right] \psi_n(\vec{r}_1 \sigma_1, \vec{r}_2 \sigma_2) = 0 \quad (2.3)$$

where E_n is the energy of the n^{th} state of the atom. The summation in equation (2.2) includes both a sum over bound spin-space states and an integration over the continuum states of the helium system. The function $F_n(\vec{r}_3, \sigma_3)$, representing the n^{th} state expansion coefficient, is a one-electron scattering wave-function. The operator A anti-symmetrizes the product functions as required by the Pauli Principle.

If the wave number of the incident electron is k_0 , in atomic units, then the one-electron scattering wave-function $F_n(\vec{r}_3, \sigma_3)$ has the asymptotic forms

$$F_0(\vec{r}_3, \sigma_3) \rightarrow \exp(i k_0 \gamma) \sigma_3 + \frac{\exp(i k_0 r_3) q_0(\theta_3) \sigma_3}{r_3} \quad (2.4)$$

and

$$F_n(\vec{r}_3, \sigma_3) \rightarrow \frac{\exp(i k_n r_3) q_n(\theta_3) \sigma_3}{r_3} \quad (2.5)$$

where the function $F_0(\vec{r}_3, \sigma_3)$ denotes the plane wave incident along the γ axis toward the target atom in the zero bound state configuration and an elastic outgoing spherical wave in the same spin state. The spin function σ_3 denotes the familiar normalized α or β spin state representing electron spin-up and spin-down, respectively. The function $F_n(\vec{r}_3, \sigma_3)$ denotes an inelastic spherical outgoing wave in the allowable spin states, σ_3 , provided k_n^2 is real. If k_n^2 is imaginary, the incident energy is less than the energy required for an internal transition of the atom to occur, and the boundary conditions, equation (2.5), describe a decaying spherical wave, the sum of which describes the polarization of the initial atomic bound

state. The constraints on the total system energy are given asymptotically as

$$\begin{aligned} E &= k_0^2 + E_0 \\ &= k_n^2 + E_n \end{aligned} \quad (2.6)$$

Once the detailed solution to the Schrodinger equation (2.1) is available, the scattering amplitudes $g_n(\theta)$ can be determined from the asymptotic boundary conditions defined by equations (2.4) and (2.5). As shown in Mott and Massey (Ref. 19), the total scattering cross-section at incident energy k_0^2 is given as

$$Q(k_0^2) = 2\pi \int_0^\infty |g_n(\theta)|^2 \sin \theta d\theta \quad (2.7)$$

Close-Coupling Approximation

Although the expansion represented by equation (2.2) is formally exact, several practical difficulties limit all scattering calculations. First, for atoms other than hydrogen or one-electron systems, the target eigen-states are not known exactly. Second, the bound target states form an infinitely denumerable set of functions. Finally, the complete set of target states must include the ionization continuum. In this case, the state index n is a continuous variable and the number, though infinite, is not denumerable.

In practice, only a relatively small number of states can be included in the expansion (2.2) and are generally carefully selected. However, a number of methods have been developed to account for those terms neglected in the expansion. The basic approach of these methods is to replace the unperturbed target state wave-functions with pseudo-state functions corresponding to the first-order perturbation of the target state by a polarizing field. These pseudo-states can be constructed in terms of the unperturbed target wave-functions or other convenient basis functions, Danburg and Karule (Ref. 21), Danburg and Geltmann (Ref. 22). The reader is referred to Mott and Massey (Ref. 19) and Nesbet (Ref. 23) for a complete discussion of

the pseudo-state method.

Since the purpose of this study is the application of a variational principle to the elastic-scattering of electrons from helium in the atomic ground state, it is convenient to adopt the simplest case of the close-coupling approximation. For incident energies of the continuum electrons less than the first excited state of helium (19 e.v.), the one-state approximation is assumed. Thus

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \vec{r}_3\sigma_3) = A \Psi_0(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) F_0(\vec{r}_3) \alpha_3 \quad (2.8)$$

where $\Psi_0(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2)$ denotes the unperturbed ground state helium wave-function, $F_0(\vec{r}_3)$ denotes the space part of the incident electron wave-function, and α_3 denotes the electron incident in the arbitrary spin-up state.

Substituting the space-spin helium wave-function and anti-symmetrizing by a cyclic perturbation of the electrons, we have

$$\begin{aligned} \Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \vec{r}_3\sigma_3) = & \Psi_0(\vec{r}_1\vec{r}_2) F_0(\vec{r}_3) (\alpha_1\beta_2 - \alpha_2\beta_1) \alpha_3 / \sqrt{2} \\ & + \Psi_0(\vec{r}_2\vec{r}_3) F_0(\vec{r}_1) (\alpha_2\beta_3 - \alpha_3\beta_2) \alpha_1 / \sqrt{2} \\ & + \Psi_0(\vec{r}_3\vec{r}_1) F_0(\vec{r}_2) (\alpha_3\beta_1 - \alpha_1\beta_3) \alpha_2 / \sqrt{2} \end{aligned} \quad (2.9)$$

where the spin function $(\alpha_1\beta_2 - \alpha_2\beta_1) \alpha_3 / \sqrt{2}$ is anti-symmetric with respect to the bound helium electrons 1 and 2 and corresponds to a doublet total spin state of the helium and incident electron.

$\Psi_0(\vec{r}_1, \vec{r}_2)$ is the space part of the helium wave-function and is symmetric with respect to electrons 1 and 2.

If we substitute the total system wave-function (2.9) into the Schrodinger equation (2.1), pre-multiply by $(\alpha_1\beta_2 - \alpha_2\beta_1) \alpha_3 \Psi_0^*(\vec{r}_1, \vec{r}_2) / \sqrt{2}$, sum over spin and integrate over \vec{r}_1 and \vec{r}_2 we obtain

$$\left[\nabla_3^2 + k_0^2 - V_{00}(r_3) \right] F_0(\vec{r}_3) = \int_0^\infty \int_0^\infty F_0(\vec{r}_1) Q_{00}(\vec{r}_1, \vec{r}_2, \vec{r}_3) d\vec{r}_1 d\vec{r}_2 \quad (2.10)$$

where

$$V_{00}(r_3) = - \int_0^\infty \int_0^\infty \left(\frac{4}{r_3} - \frac{2}{r_{12}} - \frac{2}{r_{23}} \right) |\psi_0(\vec{r}_1, \vec{r}_2)|^2 d\vec{r}_1 d\vec{r}_2 \quad (2.11)$$

and

$$\begin{aligned} Q_{00}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = & \psi_0(\vec{r}_2, \vec{r}_3) \nabla_1^2 \psi_0^*(\vec{r}_1, \vec{r}_2) + \psi_0^*(\vec{r}_1, \vec{r}_2) \nabla_2^2 \psi_0(\vec{r}_2, \vec{r}_3) \\ & + \psi_0^*(\vec{r}_1, \vec{r}_2) \psi_0(\vec{r}_2, \vec{r}_3) \left\{ \frac{4}{r_1} + \frac{4}{r_2} + \frac{4}{r_3} - \frac{2}{r_{12}} - \frac{2}{r_{13}} - \frac{2}{r_{23}} + E \right\} \\ & + \psi_0^*(\vec{r}_1, \vec{r}_2) \nabla_3^2 \psi_0(\vec{r}_2, \vec{r}_3) \end{aligned} \quad (2.12)$$

In order to obtain this result we used Green's theorem, the symmetry properties of the electrons and the equation

$$\int_0^\infty \int_0^\infty \psi_0^*(\vec{r}_1, \vec{r}_2) \left[\nabla_1^2 + \nabla_2^2 + \frac{4}{r_1} + \frac{4}{r_2} - \frac{2}{r_{12}} + E_0 \right] \psi_0(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2 = 0 \quad (2.13)$$

This condition is certainly satisfied if $\psi_0(\vec{r}_1, \vec{r}_2)$ is an exact solution to the helium equation (2.3). Unfortunately, no exact helium solution exists. However, equation (2.13) can also be satisfied if a variational wave-function for the ground state of helium is used and the ground state energy E_0 is given by the variational energy. In this study we have adopted Hylleraas' variational function given as

$$\psi_0(\vec{r}_1, \vec{r}_2) = \frac{Z^3}{\pi} \exp(-(Zr_1 + Zr_2)) \quad (2.14)$$

where $Z = 27/16$ and $E_0 = -2Z^2$ and which satisfies equation (2.13).

Equation (2.10) represents a partial integro-differential equation for the scattering function $F_0(\vec{r})$. Its exact solution, which satisfies the boundary conditions of equation (2.4), formally determines the scattering cross-sections. For low-energy scattering it is convenient to reduce the partial integro-differential equation to a set of ordinary integro-differential equations. Performing a partial wave or angular momentum expansion on the scattering function $F_0(\vec{r})$ we have

$$F_0(\vec{r}) = \frac{1}{r} \sum_{L=0}^{\infty} f_L(r) P_L(\cos \theta) \quad (2.15)$$

where $P_L(\cos \theta)$ are the Legendre polynomials. Substituting $F_0(\vec{r})$ into equation (2.10), pre-multiplying by $P_L(\cos \theta)$, and integrating over all scattering angles and using the Hylleraas helium wave-function we obtain

$$\left(\frac{d^2}{dr_3^2} + k_0^2 - V_{00}(r_3) - \frac{L(L+1)}{r_3^2} \right) f_L(r_3) = \int_0^{\infty} \int_0^{\infty} f_L(r_1) P_{00}(r_1, r_2, r_3) dr_1 dr_2 \quad (2.16)$$

where

$$V_{00}(r_3) = -4 \left(\frac{1}{r_3} + Z \right) \exp(-2Zr_3) \quad (2.17)$$

and

$$P_{00}(r_1, r_2, r_3) = \frac{16\pi^2}{(2L+1)} r_1 r_2^2 r_3 \psi_0(r_2, r_3) \psi_0(r_1, r_2) \times \left[\left\{ k_0^2 + Z^2 + (4-2Z) \left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} \right) - 2\sigma_L(r_1, r_2) - 2\sigma_L(r_2, r_3) \right\} \delta_{0L} - 2\sigma_L(r_1, r_3) \right] \quad (2.18)$$

and

$$\begin{aligned} \sigma_L(r_1, r_2) &= r_1^L / r_2^{L+1} & (r_1 < r_2) \\ &= r_2^L / r_1^{L+1} & (r_2 < r_1) \end{aligned} \quad (2.19)$$

The boundary conditions of the radial function $f_L(r)$ are

$$\begin{aligned} f_L(r) &= 0 & r \rightarrow 0 \\ f_L(r) &= \sin(k_0 r - \frac{L\pi}{2} + \eta_L) & r \rightarrow \infty \end{aligned} \quad (2.20)$$

where η_L is the energy-dependent phase shift of the L -partial wave and is determined by the exact solution to the integro-differential equation (2.16). It can be shown, Mott and Massey (Ref. 19), that the total elastic scattering cross-section at incident energy k_0^2 is

$$Q(k_0) = \frac{4\pi}{k_0^2} \sum_{L=0}^{\infty} (2L+1) \sin^2 \eta_L \quad (2.21)$$

In the case where the energy of the incident electron is small, only the zero order phase shift $\eta_0 (L=0)$ is important in the calculation of the total cross-section. This was done by Morse and Allis (Ref. 3), by numerical integration of equation (2.16).

Setting $L=0$ and defining

$$K_{00}(r_1, r_3) = \int_0^{\infty} P_{00}(r_1, r_2, r_3) dr_2 \quad (2.22)$$

we have

$$\left(\frac{d}{dr_3^2} + k_0^2 - V_{00}(r_3) \right) f_0(r_3) = \int_0^{\infty} f_0(r_1) K_{00}(r_1, r_3) dr_1 \quad (2.23)$$

where

$$\begin{aligned} K_{00}(r_1, r_3) &= 16Z^6 r_1 r_3 \exp(-Zr_1) \exp(-Zr_3) \cdot \left\{ \frac{(k_0^2 + 4Z - Z^2)}{4Z^3} \right. \\ &+ \frac{(1-Z)}{2r_1 Z^3} + \frac{(1-Z)}{2r_3 Z^3} - \frac{V_0(r_1, r_3)}{2Z^3} + \frac{\exp(-2Zr_1)}{2Z^2} + \frac{\exp(-2Zr_3)}{2Z^2} \\ &\left. + \frac{\exp(-2Zr_1)}{2r_1 Z^3} + \frac{\exp(-2Zr_3)}{2r_3 Z^3} \right\} \end{aligned} \quad (2.24)$$

III. The Variational Method

General Formulation

In order to solve variationally the S-wave integro-differential equation, we define the functional \mathcal{L} as

$$\begin{aligned} \mathcal{L} = & \int_0^{\infty} f_0^*(r_3) \left\{ \frac{d^2}{dr_3^2} + k_0^2 - V_{00}(r_3) \right\} f_0^*(r_3) dr_3 \\ & - \int_0^{\infty} f_0^*(r_3) \int_0^{\infty} f_0^*(r_1) K_{00}(r_1, r_3) dr_1 dr_3 \end{aligned} \quad (3.1)$$

where $f_0^*(r)$ is an assumed trial function.

Clearly, if $f_0^*(r)$ is an exact solution to equation (3.1), $f_0(r)$, then $\mathcal{L} = 0$. If $f_0^*(r)$ is not exact, then $\mathcal{L} = \text{constant}$. Now consider the change in \mathcal{L} if $f_0^*(r)$ is defined as

$$f_0^*(r) = f_0(r) + \delta f_0(r) \quad (3.2)$$

where $\delta f_0(r)$ is a first order deviation from the exact solution.

Substituting, the resulting change in \mathcal{L} is

$$\begin{aligned} \delta \mathcal{L} = & \int_0^{\infty} f_0(r_3) \left\{ \frac{d^2}{dr_3^2} + k_0^2 - V_{00}(r_3) \right\} \delta f_0(r_3) dr_3 \\ & - \int_0^{\infty} f_0(r_3) \int_0^{\infty} \delta f_0(r_1) K_{00}(r_1, r_3) dr_1 dr_3 + O(|\delta f_0(r)|^2) \end{aligned} \quad (3.3)$$

where the symbol $O(|\delta f_0(r)|^2)$ denotes integral terms of second order in the deviation from the exact solution.

Applying Green's theorem to the first term in equation (3.3), we have

$$\begin{aligned} \int_0^{\infty} f_0(r_3) \frac{d^2}{dr_3^2} \delta f_0(r_3) dr_3 = & \int_0^{\infty} \delta f_0(r_3) \frac{d^2}{dr_3^2} f_0(r_3) dr_3 \\ & + \left\{ f_0(r_3) \frac{d}{dr_3} \delta f_0(r_3) - \delta f_0(r_3) \frac{d}{dr_3} f_0(r_3) \right\} \Big|_0^{\infty} \end{aligned} \quad (3.4)$$

where the surface term is evaluated at the boundaries. The boundary conditions on $f_0(r)$ are given by equation (2.20) for $L=0$ as

$$\begin{aligned} f_0(r) &= 0 & r &\rightarrow 0 \\ f_0(r) &= A \sin(k_0 r + \eta_0) & r &\rightarrow \infty \end{aligned} \quad (3.5)$$

or in different form

$$f_0(r) = a_1 \sin(k_0 r) + a_2 \cos(k_0 r) \quad r \rightarrow \infty \quad (3.6)$$

where

$$\begin{aligned} a_1 &= A \cos \eta_0 \\ a_2 &= A \sin \eta_0 \end{aligned} \quad (3.7)$$

and A is a normalization constant.

The boundary conditions on the difference functions are simply

$$\begin{aligned} \delta f_0(r) &= 0 & r &\rightarrow 0 \\ \delta f_0(r) &= \delta a_1 \sin(k_0 r) + \delta a_2 \cos(k_0 r) & r &\rightarrow \infty \end{aligned} \quad (3.8)$$

Substituting for the boundary conditions, the surface term reduces as

$$\left(f_0(r_3) \frac{d}{dr_3} \delta f_0(r_3) - \delta f_0(r_3) \frac{d}{dr_3} f_0(r_3) \right) \Big|_0^\infty = +a_2 \delta a_1 k_0 - a_1 \delta a_2 k_0 \quad (3.9)$$

If we impose on the normalization constant A , the condition

$$\delta A = 0 \quad (3.10)$$

then it follows that

$$+a_2 \delta a_1 k_0 - a_1 \delta a_2 k_0 = -k_0 A^2 \delta \eta_0 \quad (3.11)$$

and the resultant change in the functional \mathcal{L} is

$$\begin{aligned} \delta \mathcal{L} = & -k_0 A^2 \delta \eta_0 + \int_0^\infty \delta f_0(r) \left\{ \frac{d^2}{dr^2} + k_0^2 - V_{00}(r) \right\} f_0(r) dr \\ & - \int_0^\infty f_0(r_3) \int_0^\infty \delta f_0(r_1) K_{00}(r_1, r_3) dr_1 dr_3 + O(|\delta f_0(r)|^2) \end{aligned} \quad (3.12)$$

Since the kernel function $K_{00}(r_1, r_3)$ defined by equation (2.24) is symmetric in r_1 and r_3 we may interchange the order of integration and interchange the indices in the third term of equation (3.12).

Thus we have

$$\int_0^\infty f_0(r_3) \int_0^\infty \delta f_0(r_1) K_{00}(r_1, r_3) dr_1 dr_3 = \int_0^\infty \delta f_0(r_3) \int_0^\infty f_0(r_1) K_{00}(r_1, r_3) dr_1 dr_3 \quad (3.13)$$

Substituting into equation (3.12) we have

$$\delta \mathcal{L} = -k_0 A^2 \delta \eta_0 + O(|\delta f_0(r)|^2) \quad (3.14)$$

where the differential and integral terms vanish since $f_0(r)$ is an exact solution to the integro-differential equation (3.1).

Since the second order term can be forced vanishing small by choosing more and more complex trial functions $f_0^{\epsilon}(r_3)$ which better approximates the exact solution $f_0(r_3)$, we have

$$\delta(\mathcal{L} + k_0 A^2 \eta_0) = 0 \quad (3.15)$$

Thus the functional $(\mathcal{L} + k_0 A^2 \eta_0)$ is stationary provided $\delta A = 0$.

Since the condition $\delta A = 0$ represents a constraint on the variational principle it can conveniently be incorporated into the stationary equation (3.15) by use of a Lagrange multiplier.

From equation (3.7) we have

$$\begin{aligned} A^2 &= a_1^2 + a_2^2 \\ \eta_0 &= \tan^{-1}(a_2/a_1) \end{aligned} \quad (3.16)$$

If we require the normalization of the asymptotic solution, equation (3.5) as $A=1$, which satisfies the condition $dA=0$, then the constraint equation becomes

$$a_1^2 + a_2^2 - 1 = 0 \quad (3.17)$$

Substituting equation (3.16) into (3.15), and introducing a free parameter $\lambda/2$, a Lagrange multiplier, the stationary functional can be written as

$$\Pi = \mathcal{L} + k_0(a_1^2 + a_2^2) \tan^{-1}(a_2/a_1) - \frac{\lambda}{2}(a_1^2 + a_2^2 - 1) \quad (3.18)$$

Matrix Variational Method

Let $f_0^T(r)$ denote a trial function defined as

$$f_0^T(r) = \sum_1^N a_n \phi_n(r) \quad (3.19)$$

where $\{\phi_n(r)\}$ is an assumed set of functions, and $\{a_n\}$ a set of undetermined coefficients. The conditions on the function set are

$$\phi_1(r) = \sin(k_0 r) \quad (3.20)$$

$$\phi_2(r) = \cos(k_0 r)(1 - \exp(-\alpha_0 r))$$

and

$$\begin{aligned} \{\phi_n(r)\} &= 0 & r &= 0 & (n \geq 3) \\ \{\phi_n(r)\} &= 0 & r &\rightarrow \infty & (n \geq 3) \end{aligned} \quad (3.21)$$

where α_0 is an assumed positive definite parameter. We assume that

the trial function, equation (3.19) is an approximate solution to the integro-differential equation (2.23). Clearly by construction the trial function satisfies the boundary conditions of the exact solution, equation (3.6).

If we substitute the trial function into the functional equation (3.1), and perform the differential and integral operations, the functional \mathcal{L} becomes

$$\mathcal{L} = \sum_{n=1}^N \sum_{m=1}^N a_n (A_{nm} - B_{nm}) a_m \quad (3.22)$$

where

$$A_{nm} = \int_0^{\infty} \phi_n(r_3) \left\{ \frac{d^2}{dr_3^2} + k_0^2 - V_{00}(r_3) \right\} \phi_m(r_3) dr_3 \quad (3.23)$$

and

$$B_{nm} = \int_0^{\infty} \phi_n(r_3) \int_0^{\infty} \phi_m(r_1) K_{00}(r_1, r_3) dr_1 dr_3 \quad (3.24)$$

Since the functions $\{\phi_n(r)\}$ are known, the A and B elements are numbers corresponding to a given value of the electron energy k_0^2 . The functional \mathcal{L} at a given electron energy reduces to a numerical set of terms in the undetermined coefficients a_n . Thus the functional which is stationary under variations is

$$\mathcal{I} = \sum_{n=1}^N \sum_{m=1}^N a_n (A_{nm} - B_{nm}) a_m + k_0 (a_1^2 + a_2^2) \tan^{-1} \left(\frac{a_2}{a_1} \right) - \frac{\lambda}{2} (a_1^2 + a_2^2 - 1) \quad (3.25)$$

If we vary the functional with respect to the parameter set $\{a_n\}$ we obtain a set of N equations defined by

$$\frac{\partial \mathcal{I}}{\partial a_n} = 0 \quad (1 \leq n \leq N) \quad (3.26)$$

Performing the differentiation, the resulting set of equations

in matrix form is

$$(\bar{D} - k_0 \bar{B}) \bar{a} - (\lambda - 2k_0 \eta_0) \bar{M} \bar{a} = 0 \quad (3.27)$$

where \bar{D} is an $N \times N$ symmetric matrix whose elements are

$$D_{nm} = (A_{nm} - B_{nm}) + (A_{mn} + B_{mn}) \quad (3.28)$$

\bar{B} is an $N \times N$ matrix with elements $B_{12} = 1$, $B_{21} = -1$ and the set $\{B_{nm} = 0\}$, \bar{a} is the $N \times 1$ column matrix whose element set is $\{a_n\}$ and \bar{M} is an $N \times N$ matrix with elements $M_{11} = M_{22} = 1$ and $\{M_{nm} = 0\}$.

Formally, equation (3.27) represents an $N \times N$ linear matrix problem which can be solved for the complete set of coefficients, $\{a_n\}$. However, only the coefficients a_1 and a_2 have physical significance for determining the scattering phase shift, equation (3.16), and thus the collisional cross-section. It is convenient therefore to reduce the $N \times N$ linear matrix problem to a 2×2 eigen-value problem.

Let X be a sub-set of the column matrix \bar{a} composed of two elements a_1 and a_2 . Similarly, let Y be a sub-set column composed of $N-2$ elements $a_3 \cdots a_N$. Thus

$$\bar{a} = \begin{pmatrix} X \\ Y \end{pmatrix} \quad (3.29)$$

Defining

$$\mu = \lambda - 2k_0 \eta_0 \quad (3.30)$$

equation (3.27) becomes

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \mu \begin{pmatrix} X \\ 0 \end{pmatrix} \quad (3.31)$$

where C_{11} is a 2×2 array consisting of the four elements: D_{11} , $D_{12} - k_0$, $D_{21} + k_0$, and D_{22} . The term C_{12} is a two row by N column array containing the element sets $\{D_{1n}\}$ and $\{D_{2n}\}$ for $(3 \leq n \leq N)$. Similarly C_{21} is an N row by two column array containing the elements $\{D_{n1}\}$ and $\{D_{n2}\}$ for $(3 \leq n \leq N)$. In particular, C_{21} is the transpose of C_{12} . Finally, C_{22} is an $(N-2) \times (N-2)$ symmetric array composed of the elements $\{D_{nm}\}$ $n, m \geq 3$.

Expanding the matrix equation (3.30) we have

$$\begin{aligned} C_{11}X + C_{12}Y &= \mu X \\ C_{21}X + C_{22}Y &= 0 \end{aligned} \quad (3.32)$$

Operating on the lower set of matrix equations by the inverse matrix of the C_{22} array, we have

$$Y = -C_{22}^{-1} C_{21} X \quad (3.33)$$

Substituting for Y we obtain a 2×2 eigen-value problem

$$(C_{11} - C_{12} C_{22}^{-1} C_{21})X = \mu X \quad (3.34)$$

Expanding out the C_{11} elements the eigen-value problem becomes

$$\begin{bmatrix} (D_{11} - E_{11}) & (D_{12} - E_{12} - k_0) \\ (D_{21} - E_{21} + k_0) & (D_{22} - E_{22}) \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \mu \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad (3.35)$$

where we have defined the value of the E elements as

$$E_{nm} = C_{12} C_{22}^{-1} C_{21} \Big|_{nm} \quad \begin{matrix} n=1,2 \\ m=1,2 \end{matrix} \quad (3.36)$$

and denotes the nm elements of the $C_{12} C_{22}^{-1} C_{21}$ matrix operation.

The characteristic equation for the eigen-values μ is simply

$$\begin{aligned} \mu^2 - \mu \{ (O_{11} - E_{11}) + (O_{22} - E_{22}) \} + \{ (O_{11} - E_{11})(O_{22} - E_{22}) \\ - (O_{12} - E_{12} - k_0)(O_{21} - E_{21} + k_0) \} = 0 \end{aligned} \quad (3.37)$$

which can be solved by elementary means.

The solution to equation (3.37) yields two eigen-values, μ_1 and μ_2 since the characteristic equation is quadratic in μ . Similarly there exist two eigen-vector solutions, X_1 and X_2 , as well as two values of the phase shifts η_1 and η_2 for each value of the incident energy.

In practice it is not difficult, in general, to select which values of the phase shift correspond to a physical solution to the scattering problem. This is due to the fact that the phase shifts are defined as the arc tangents of the ratios of the components of the eigen-vectors, equation (3.16). Thus one set of phase shifts will exhibit a uniform and continuous behavior as a function of energy, while the second set of phase shifts exhibits a strongly divergent behavior in energy. Although both sets of phase shifts represent the formal solution to the quadratic equation, the diverging set of phase shifts can be rejected as the physical solution to the scattering problem.

However, equation (3.7) presents a far more difficult problem for specific regions of the electron energy. Since $C_{12} \neq C_{21}^T$, the roots of the characteristic equation can be complex. Since the scattering phase shifts are real for all values of the electron energy less than the excitation energy of the helium atom, the variational method will fail. In this case both solutions to the characteristic equation yield non-physical results.

Another problem results due to the quadratic nature of the characteristic equation and the continuous dependence of the solutions on the incident energy, k_0^2 . While over a broad range of the energy spectrum only one set of phase shifts represents the physical solution to the scattering problem, for different energy regions the physical set can change. Thus we can expect a small energy region in which both sets of phase shifts are simultaneously diverging. In these regions the physical phase shift must be obtained by averaging the two. It must be emphasized that there is no physical significance to the anomalous behavior of the phase shifts as a function of incident electron energies. In fact, the anomalous behavior is simply an artifact of the variational method of calculation applied to the continuum scattering problem.

In Chapter IV we will develop a computational algorithm for the variational calculation using Slater-type trial functions for the trial function set $\{\phi_n(r)\}, n \geq 3$. In particular we will also discuss an interpolation technique to obtain values for the phase shifts at the anomalous energy values.

IV. The Variational Calculation Algorithm

Slater-Type Functions

The first step in the variational calculation is the selection of a specific set of basis functions to represent the trial solution, $f_0^{\pm}(r)$. Clearly, the basis functions $\phi_1(r)$ and $\phi_2(r)$, defined by the equations (3.20), are constructed in order to satisfy the boundary conditions of the exact solution to the integro-differential equation, equation (2.23). However, the conditions imposed on the basis set of functions for $n \geq 3$ are simply that they vanish at the boundaries, equation (3.21). A particularly simple set of functions which satisfy the conditions are the Slater-type Functions defined as

$$\phi_n(r) = r \exp(-\beta_n r) \quad (4.1)$$

where β_n is a positive number which is different for each functional term in the expansion, equation (3.19). Thus the assumed form of the trial wave-function is

$$f_0^{\pm}(r) = a_1 \sin(k_0 r) + a_2 \cos(k_0 r)(1 - \exp(-a_0 r)) + \sum_{n=3}^N a_n r \exp(-\beta_n r) \quad (4.2)$$

Substituting equation (4.2) into equations (3.23) and (3.24) we can obtain explicitly the matrix elements A_{nm} and B_{nm} . Appendix I is a compilation of the A_{nm} matrix elements. Appendix II is a compilation of the B_{nm} matrix elements. Appendix III is a compilation and an evaluation of the definite integrals in which the elements A_{nm} and B_{nm} are expressed. Since the evaluation of the matrix elements is particularly tedious, the choice of the Slater-Type Functions was made to minimize the chance for error involved in the evaluation. In addition, the definite integrals resulting from the differentiation and integration of the functions

have, in general, simple closed-form solutions. Clearly there is little restriction on the form of the basis set for $\{\phi_n(r)\}$, $n \geq 3$. However, in order to take advantage of the Variational Method as a labor saving technique for scattering calculations, there exists, in practice, a pragmatic trade-off in the selection of the basis set.

Clearly, with the set of matrix elements given in the appendices, we are in a position to generate a computational algorithm to calculate the S-wave phase shift for the elastic scattering of electrons from helium in the atomic ground state.

Computational Algorithm

STEP I: Initialization of Parameters

There are two types of numerical parameters needed in the calculation. First, the values for k_0 and Z denoting the wave-number of the incident electron and the ground state energy of the helium atom relative to the first ionization continuum, $E_0 = -Z^2$ (atomic units). For the Hylleraas wave-function, equation (2.14), the first continuum is $E_0 = -2.9476$, which restricts the values of k_0 between $0 < k_0 < 1.68$. Since we have neglected the contributions of the excited states of helium, the values taken by k_0^2 must be restricted to less than the energy of the first excited state of the target atom. Thus we have $Z = 1.607$ and $0 < k_0 \lesssim 1.3$.

The second set of parameters required are those defined by the basis set, α_0 and the set $\{\beta_n\}$, depending on the number of Slater-Type Functions assumed. Sinfailam and Nesbet (Ref. 12) have had particular success in the more complex anomaly-free Variational Method with a decreasing geometric progression of exponents. Although this selection is difficult to justify on mathematical grounds, we will assume that the decreasing geometric progression represents a starting point in the calculation. Clearly, accurate cross-sections will result only after several different runs are made using different distributions of the parameters $\{\beta_n\}$. To initiate the calculation,

the following set of parameters are defined $\alpha_0 = 1$, $\beta_2 = 2$,
 $\beta_n = (\beta_{n-1})/2$, for $n > 3$.

STEP II: Calculation of the Matrix Elements

Once the numerical values Z , k_0 , α_0 , β_2 , β_4 ... β_N are specified, the matrix elements A_{nm} and B_{nm} can be calculated explicitly using the Appendices and the formulae for the evaluation of the definite integrals, Appendix III.

STEP III: Construct the D_{nm} Matrix

Once the matrix elements A_{nm} and B_{nm} are known, we can construct an auxiliary matrix D_{nm} given by equation (3.28). If we set $D'_{12} = D_{12} - k_0$ and $D'_{21} = D_{21} + k_0$, the simultaneous equations are defined, equation (3.31). For illustrative purposes we will assume a two-free parameter trial function which produces a 4×4 matrix set. Thus equation (3.31) becomes

$$\begin{bmatrix} D_{11} & D'_{12} & D_{13} & D_{14} \\ D'_{21} & D_{22} & D_{23} & D_{24} \\ D_{31} & D_{32} & D_{33} & D_{34} \\ D_{41} & D_{42} & D_{43} & D_{44} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \mu \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} \quad (4.3)$$

where

$$C_{11} = \begin{pmatrix} D_{11} & D'_{12} \\ D'_{21} & D_{22} \end{pmatrix} \quad (4.4)$$

$$C_{22} = \begin{pmatrix} D_{33} & D_{34} \\ D_{43} & D_{44} \end{pmatrix} \quad (4.5)$$

$$C_{12} = \begin{pmatrix} D_{13} & D_{14} \\ D_{23} & D_{24} \end{pmatrix} \quad \text{and} \quad C_{21} = C_{12}^T \quad (4.6)$$

In fact, the C_{22} matrix is independent of the number of basis functions used in the expansion of the trial function $f_0^k(r)$.

STEP IV: Calculate the E Matrix

At this point the 2×2 eigen-value problem is set up, equation (3.35). The most difficult part of the program, from a numerical point, is the operation $C_{12} C_{22}^{-1} C_{12}^T$, to yield a 2×2 matrix with elements

$$\begin{aligned} E_{11} &= C_{12} C_{22}^{-1} C_{12}^T I_{11} \\ E_{12} &= C_{12} C_{22}^{-1} C_{12}^T I_{12} \\ E_{21} &= C_{12} C_{22}^{-1} C_{12}^T I_{21} \\ E_{22} &= C_{12} C_{22}^{-1} C_{12}^T I_{22} \end{aligned} \quad (4.7)$$

Clearly in the case illustrated, this only requires obtaining the inverse of the 2×2 matrix, and can be accomplished by elementary means, provided $\text{DET } C_{22} \neq 0$. For the general N -trial function case, we require the inverse of a $N-2 \times N-2$ matrix. In fact, the speed and efficiency of performing the C_{22}^{-1} matrix operation represents a pragmatic bound on the number of basis functions used or the range of incident electron energy spanned in a single machine run. Clearly, if $\text{DET } C_{22} = 0$, which is a preliminary requirement for the C_{22}^{-1} operation, the Matrix Variational Method completely fails to yield a phase shift at the specific value of k_0^2 . In this case the trial function assumed does not represent the exact solution to the integro-differential equation to first order and the stationary principle must be suspect. Clearly, additional terms must be added to $f_0^k(r)$ and the particular energy region around k_0^2 studied in a later machine run. In practice, if $\text{DET } C_{22} = 0$, a simple print of the singular region is only required. A return to STEP II with an incremental increase in the value of k_0^2 removes the calculation from the singularity and the program proceeds.

STEP V: Solving the Eigen-Value Problem

All the elements are now available to solve the eigen-value problem, equation (3.37), and which is of the form

$$\mu^2 + b\mu + c = 0 \quad (4.8)$$

which has the solution

$$\mu = \frac{-b \pm \sqrt{b^2 - 4c}}{2} \quad (4.9)$$

and yields the real eigen-values μ_1 and μ_2 , provided $b^2 > 4c$. In this case the eigen-values are substituted back into equation (3.35) and the real components of the eigen-vectors $(a_1, a_2)_1$ and $(a_1, a_2)_2$ are determined. From these, the needed phase shifts are calculated as $\eta_1 = \tan^{-1}(a_2/a_1)_1$ and $\eta_2 = \tan^{-1}(a_2/a_1)_2$.

Figure 1 is a schematic plot of the real eigen-values η_1 and η_2 as a function of k_0^2 for electron scattering from hydrogen, Shankland (Ref. 16). Although the basis set used by Shankland were Gauss-type functions, the general characteristic of the solutions, using the Variational Method, are independent of the basis set. Thus Figure 1 illustrates the general nature of the solution to the eigen-value problem.

From the figure, it is clear that at a given wave-number k_0 , only one phase shift has converged to the exact solution to the scattering equation. The other phase shift is divergent. In practice, a simple print and/or plot of the values η_1 and η_2 as a function of k_0 is sufficient to determine accurately the physical phase shift over the entire energy spectrum.

However, there exist anomalous regions near $k_0 \sim .1$ and $k_0 \sim .7$ where neither solution η_1 or η_2 converged to the exact solution. Similarly, there exists another region $k_0 \sim 1.5$ where $b^2 < 4c$ and the roots of the eigen-value problem are imaginary. Clearly, if

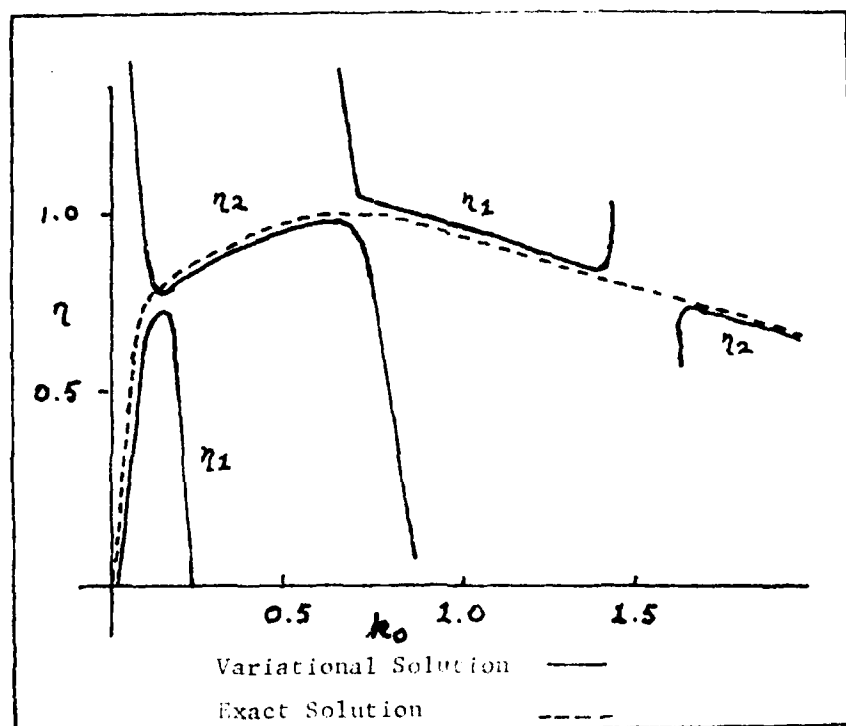


Figure 1. The Phase Shifts η_1 and η_2 for Elastic Scattering from Hydrogen, as a Function of Incident Wave-Number k_0 .

high accuracy of the phase shifts is not required in the anomalous regions, then simple graphical or polynomial fits can be used to estimate the value of the phase shifts. If high accuracy is required, a more powerful interpolation technique is needed.

Interpolation Technique

Since the general location and nature of the anomalies are known, a second machine run is required to study the anomaly in detail. In this case the range on k_0 is restricted to the anomalous region.

Real Phase Shifts

Shankland (Ref. 16) proposed an empirical technique to obtain accurate phase shifts in the anomalous regions, where η_1 and η_2 are real, based on the Stationary Principle. Clearly, the entire development of the Variational Method is based on the fact that the functional $\Pi = \mathcal{L} + A^2 k_0 \eta$, equation (3.15), is stationary with respect to variations of the functional. Thus the value of the functional Π has two real values defined as

$$\Pi_1 = \mathcal{L}_1 + A^2 k_0 \eta_1 \quad (4.10)$$

$$\Pi_2 = \mathcal{L}_2 + A^2 k_0 \eta_2 \quad (4.11)$$

Defining the weighed average of the functional as

$$\bar{\Pi} = \frac{\mathcal{L}_2 \Pi_1 - \mathcal{L}_1 \Pi_2}{\mathcal{L}_2 - \mathcal{L}_1} \quad (4.12)$$

we have

$$\bar{\Pi} = \bar{\mathcal{L}} + A^2 k_0 \bar{\eta} \quad (4.13)$$

However, since $\bar{x}=0$ we finally have

$$\bar{\eta} = \frac{x_2 \eta_1 - x_1 \eta_2}{x_2 - x_1} \quad (4.14)$$

In order to calculate numerically the values x_1 and x_2 we require the entire set of coefficients $a_1, a_2 \dots a_n$, equation (3.22). Fortunately, much of the information required is already calculated as part of the eigen-value problem. In fact, the $(a_3 \dots a_n)$ set of coefficients can be obtained by equation (3.32). Thus the coefficient sets $(a_3 \dots a_n)$ for each given eigen-vector set $(a, a_2)_1$ and $(a, a_2)_2$ are the solutions of

$$(\mathbb{I} - C_{22}^{-1} C_{12}^T (C_{11} - \mu_1 \mathbb{I})^{-1} C_{12}) Y_2 = 0 \quad (4.15)$$

$$(\mathbb{I} - C_{22}^{-1} C_{12}^T (C_{11} - \mu_2 \mathbb{I})^{-1} C_{12}) Y_2 = 0 \quad (4.16)$$

where the matrix operation $C_{22}^{-1} C_{12}^T$ is calculated as sub-section of the 2×2 eigen-value calculation. Thus the values of x_1 and x_2 can be determined.

Imaginary Phase Shifts

In this particular case, $b^2 < 4c$ and the roots of the eigen-value problem are imaginary, equation (4.9). Thus the variational method fails to predict a real phase shift in this anomalous region.

Since the two roots are complex conjugates of each other, $\mu_1 = \mu_2^*$, the components of the eigen-vectors will also be complex conjugates: $X_1 = X_2^*$. In order to calculate the complex phase shifts we require a formula for the arctangent of an imaginary number. Let $z = x + iy$ where x and y are real. Then Abramowitz

and Segun (Ref. 25) show

$$\eta = n\pi + \frac{1}{2} \tan^{-1} \left(\frac{2x}{1-x^2-y^2} \right) + \frac{i}{4} \ln \left(\frac{x^2+(y+1)^2}{x^2+(y-1)^2} \right) \quad (4.17)$$

thus we find $\eta_1 = \eta_2^*$. Since $x_2 = x_1^*$, substituting into equation (4.4), we have

$$\bar{\eta}(\text{REAL}) = \frac{\text{Im}(x_1^* \eta_1)}{\text{Im}(x_1^*)} \quad (4.18)$$

which represents an interpolation formula for obtaining the real phase shift in the anomalous region of the complex eigen-values.

In Figure 2 we will outline the basic steps required to compute the phase shifts for elastic scattering in algorithm form.

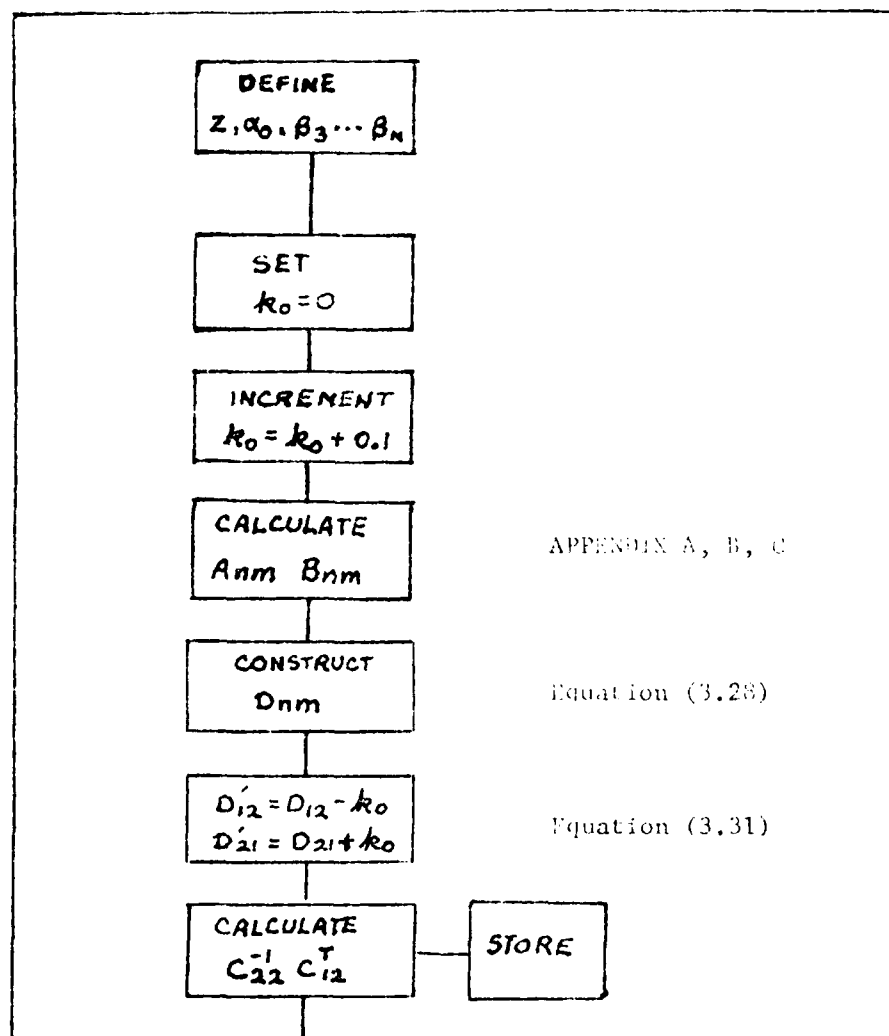


Figure 2. Algorithm for the Calculation of the S-Wave Phase Shift for Elastic Electron Helium Scattering (continued).

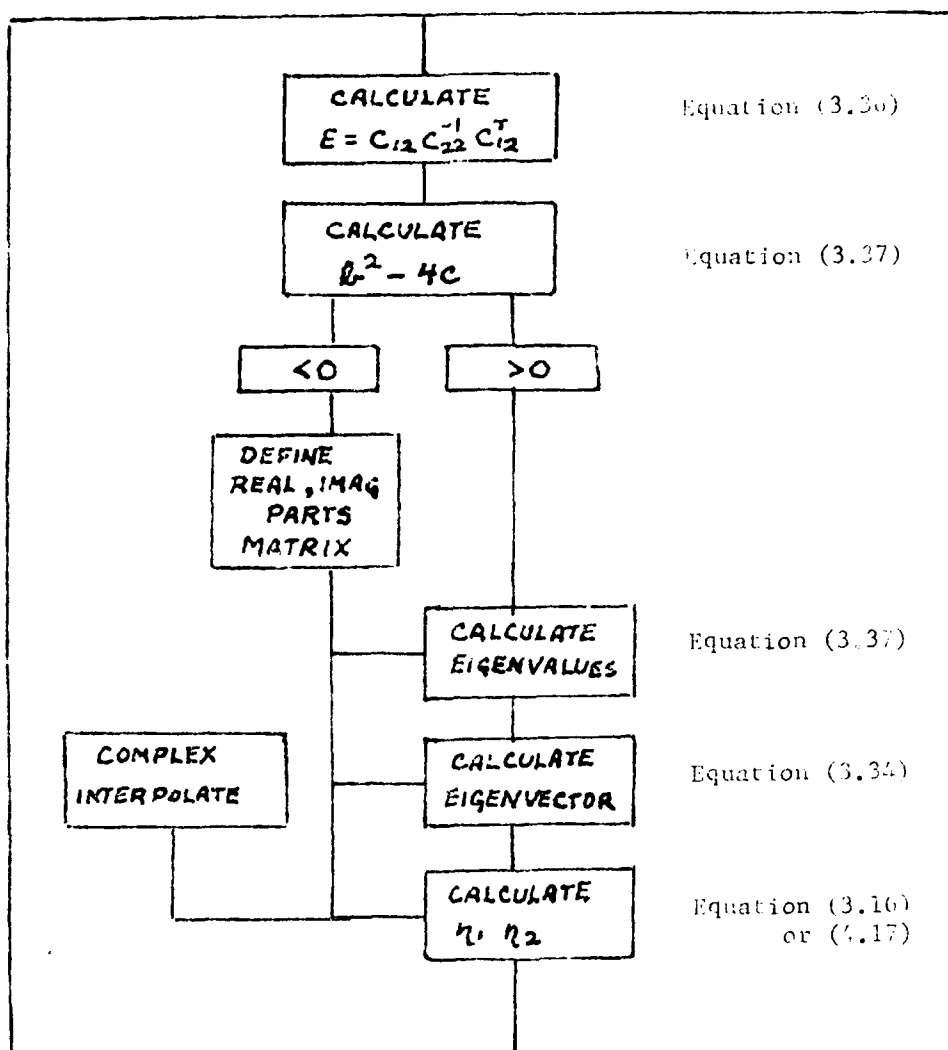


Figure 2. Algorithm for the Calculation of the S-Wave Phase Shift for Elastic Electron Helium Scattering (continued).

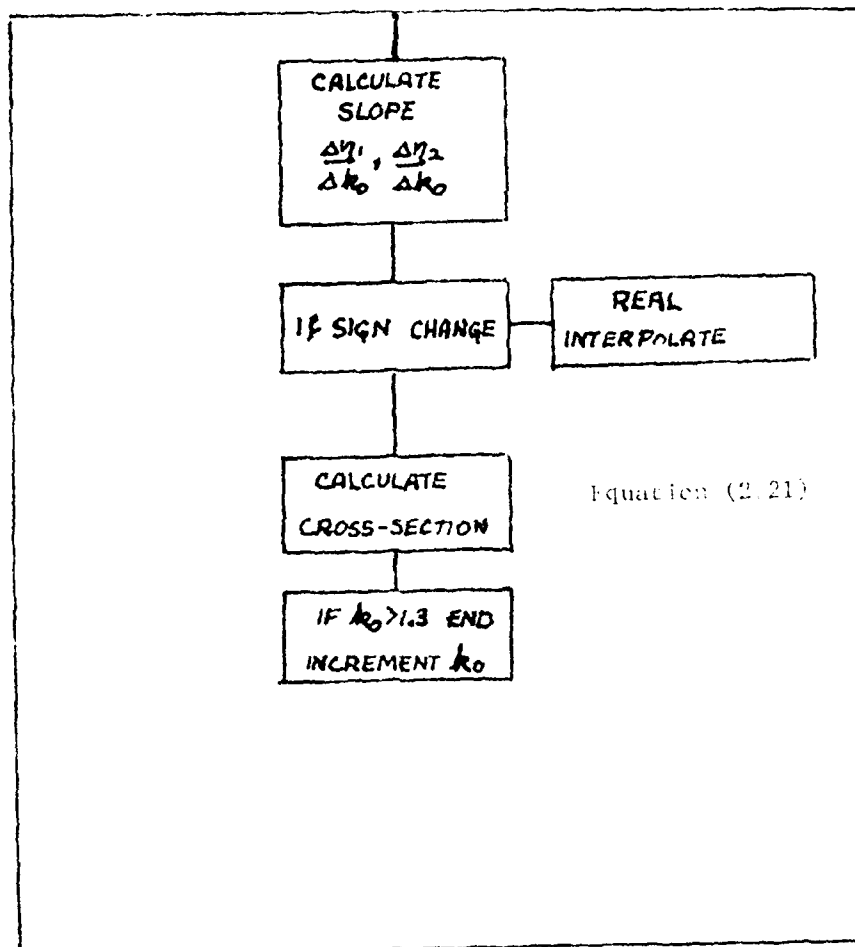


Figure 2. Algorithm for the calculation of the S-Wave Phase Shift for Elastic Electron Helium Scattering.

V. Conclusion

The object of this thesis was to theoretically formulate the Shankland Variational Method for application to the electron-helium elastic scattering problem. It was found that the scattering problem reduces, in the limit of low electron incident energy, to solving an integro-differential equation.

Instead of formally solving the differential equation, a variational approach was used to approximate the exact solution. The results obtained by applying the variational stationary principle were formulated into a general matrix problem. It was shown that the matrix problem reduces to a 2×2 matrix eigen-value problem.

An algorithm was developed to calculate the phase shifts for the scattering electron at incident energy k_0^2 , by solving the eigen-value problem. An interpolating technique was discussed which can extract the phase shifts when the eigen-value problem gives anomalous results.

It appears from the theoretical formalism that the Matrix Variational Method provides a relatively simple technique for solving complicated scattering problems. The author suggests that further work be directed toward implementing the algorithm numerically and comparing the results with known numerical solutions of the integro-differential equation. Although the physical limitations of the theory preclude comparing the results with experimental measurements, the author suggests that further work be performed to develop the technique for polarized orbitals and inelastic collisions.

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APPENDIX A The A Matrix Elements

In this appendix we list the **A** matrix elements defined by equation (3.23) and using the trial wave-function defined by equation (4.2).

$$A_{11} = \frac{4Z}{k_0} \Pi_1(2Z/k_0) + 4 \Pi_2(2Z/k_0)$$

$$A_{12} = - \left[\frac{\alpha_0^2}{k_0} \Pi_3(\alpha_0/k_0) + 2\alpha_0 \Pi_1(\alpha_0/k_0) + 4 \left\{ \Pi_4((\alpha_0+2Z)/k_0) - \Pi_4(2Z/k_0) \right\} \right. \\ \left. + \frac{4Z}{k_0} \left\{ \Pi_3((\alpha_0+2Z)/k_0) - \Pi_3(2Z/k_0) \right\} \right]$$

$$A_{1N} = \frac{(\beta_n^2 + k_0^2)}{k_0^2} \Pi_5(\beta_n/k_0) - \frac{2\beta_n}{k_0} \Pi_6(\beta_n/k_0) + \frac{4}{k_0} \Pi_6((\beta_n+2Z)/k_0) \\ + \frac{4Z}{k_0^2} \Pi_5((\beta_n+2Z)/k_0)$$

$$A_{21} = 4 \Pi_4(2Z/k_0) - 4 \Pi_4((2Z+\alpha_0)/k_0) + \frac{4Z}{k_0} \Pi_3(2Z/k_0) \\ - \frac{4Z}{k_0} \Pi_3((2Z+\alpha_0)/k_0)$$

$$A_{22} = - \left[\frac{\alpha_0^2}{k_0} \left\{ \Pi_7(\alpha_0/k_0) - \Pi_7(2\alpha_0/k_0) \right\} + 2\alpha_0 \left\{ \Pi_3(\alpha_0/k_0) - \Pi_3(2\alpha_0/k_0) \right\} \right. \\ - 4 \left\{ \ln\left(\frac{2Z+\alpha_0}{2Z}\right) - \Pi_7(2Z/k_0) + \Pi_7((2Z+\alpha_0)/k_0) \right\} \\ + 4 \left\{ \ln\left(\frac{2Z+2\alpha_0}{2Z+\alpha_0}\right) - \Pi_7((2Z+\alpha_0)/k_0) + \Pi_7((2Z+2\alpha_0)/k_0) \right\} \\ \left. - \frac{4Z}{k_0} \left\{ \Pi_7(2Z/k_0) - 2\Pi_7((2Z+\alpha_0)/k_0) + \Pi_7((2Z+2\alpha_0)/k_0) \right\} \right]$$

$$A_{2n} = \left[\frac{(\beta_n^2 + k_0^2)}{k_0^2} \{ \Pi_8(\beta_n/k_0) - \Pi_8((\alpha_0 + \beta_n)/k_0) \} \right. \\
+ \frac{2\beta_n}{k_0} \{ \Pi_9((\beta_n + \alpha_0)/k_0) - \Pi_9(\beta_n/k_0) \} \\
+ \frac{4}{k_0} \{ \Pi_9((\beta_n + 2Z)/k_0) - \Pi_9((\beta_n + \alpha_0 + 2Z)/k_0) \} \\
\left. + \frac{4Z}{k_0} \{ \Pi_9((\beta_n + 2Z)/k_0) - \Pi_9((\beta_n + \alpha_0 + 2Z)/k_0) \} \right]$$

$$A_{n1} = \frac{4}{k_0} \Pi_6((\beta_n + 2Z)/k_0) + \frac{4Z}{k_0^2} \Pi_5((\beta_n + 2Z)/k_0)$$

$$A_{n2} = - \left[\frac{\alpha_0^2}{k_0} \Pi_8((\beta_n + \alpha_0)/k_0) + \frac{2\alpha_0}{k_0} \Pi_5((\beta_n + \alpha_0)/k_0) \right. \\
+ \frac{4Z}{k_0^2} \{ \Pi_8((\beta_n + \alpha_0 + 2Z)/k_0) - \Pi_8((\beta_n + 2Z)/k_0) \} \\
\left. - \frac{4}{k_0} \{ \Pi_9((\beta_n + 2Z)/k_0) - \Pi_9((\beta_n + \alpha_0 + 2Z)/k_0) \} \right]$$

$$A_{nm} = \left[\frac{+2(\beta_m^2 + k_0^2)}{(\beta_n + \beta_m)^3} - \frac{2\beta_m}{(\beta_n + \beta_m)^2} + \frac{4}{(\beta_n + \beta_m + 2Z)^2} \right. \\
\left. + \frac{4Z}{(\beta_n + \beta_m + 2Z)^3} \right]$$

$$A_{nn} = \left[\frac{(\beta_n^2 + k_0^2)}{4\beta_n^3} - \frac{1}{4\beta_n} + \frac{1}{(\beta_n + Z)^2} + \frac{Z}{2(\beta_n + Z)^3} \right]$$

APPENDIX 2 The B Matrix Elements

In this appendix we list the B matrix elements defined by equation (3.24) and using the trial wave-function defined by equation (4.2).

$$B_{11} = \frac{8Z^3}{k_0^3} \Pi_5(Z/k_0) \left[\frac{(k_0^2 + 4Z - Z^2)}{2k_0} \Pi_5(Z/k_0) + \frac{2Z}{k_0} \Pi_5(3Z/k_0) \right. \\ \left. + 2 \Pi_6(3Z/k_0) + (1 - 2Z) \Pi_6(Z/k_0) + \Pi_3(2Z/k_0) \right] \\ + \frac{8Z^3}{k_0^3} \Pi_9(Z/k_0) \Pi_1(2Z/k_0)$$

$$B_{12} = \frac{8Z^3}{k_0^3} \left[\frac{(k_0^2 + 4Z - Z^2)}{2k_0} \Pi_5(Z/k_0) \{ \Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \} \right. \\ + (1 - Z) \Pi_5(Z/k_0) \{ \Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \} \\ + (1 - Z) \Pi_6(Z/k_0) \{ \Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \} \\ + (Z/k_0) \Pi_5(Z/k_0) \{ \Pi_9(3Z/k_0) - \Pi_9((3Z + \alpha_0)/k_0) \} \\ + (Z/k_0) \Pi_5(3Z/k_0) \{ \Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \} \\ + \Pi_5(Z/k_0) \{ \Pi_9(3Z/k_0) - \Pi_9((3Z + \alpha_0)/k_0) \} \\ + \Pi_6(3Z/k_0) \{ \Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \} \\ + \{ \Pi_9(Z/k_0) \Pi_3(2Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \Pi_3((2Z + \alpha_0)/k_0) \} \\ + \{ \Pi_5((Z + \alpha_0)/k_0) \Pi_1((2Z + \alpha_0)/k_0) - \Pi_5(Z/k_0) \Pi_1(2Z/k_0) \} \\ \left. + \{ \Pi_9((Z + \alpha_0)/k_0) \Pi_6(2Z + \alpha_0)/k_0 - \Pi_9(Z/k_0) \Pi_6(Z/k_0) \} \right]$$

$$\begin{aligned}
B_{1n} = \frac{8Z^3}{k_0} & \left[\frac{\Pi_5(Z/k_0)}{k_0} \left\{ \frac{(k_0^2 + 4Z - Z^2)}{(Z + \beta_n)^3} + \frac{(1-Z)}{k_0(Z + \beta_n)^2} + \frac{2Z}{k_0(3Z + \beta_n)^3} \right. \right. \\
& + \frac{1}{k_0(3Z + \beta_n)^2} \left. \right\} + \frac{2Z \Pi_5(3Z/k_0)}{k_0(Z + \beta_n)^3} + \frac{2\Pi_6(3Z/k_0)}{(Z + \beta_n)^3} \\
& - \frac{2Z \Pi_6(Z/k_0)}{(Z + \beta_n)^3} + \frac{\Pi_5((2Z + \beta_n)/k_0)}{k_0(Z + \beta_n)^2} + \frac{2\Pi_6((2Z + \beta_n)/k_0)}{(Z + \beta_n)^3} \left. \right]
\end{aligned}$$

$$\begin{aligned}
B_{21} = \frac{8Z^3}{k_0^3} & \left[\frac{(k_0^2 + 4Z - Z^2)}{2k_0} \Pi_5(Z/k_0) \left\{ \Pi_8(Z/k_0) - \Pi_8((Z + \alpha_0)/k_0) \right\} \right. \\
& + (1-Z) \Pi_5(Z/k_0) \left\{ \Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0) \right\} \\
& + (1-Z) \Pi_6(Z/k_0) \left\{ \Pi_8(Z/k_0) - \Pi_8((Z + \alpha_0)/k_0) \right\} \\
& + (Z/k_0) \Pi_5(Z/k_0) \left\{ \Pi_8(3Z/k_0) - \Pi_8((3Z + \alpha_0)/k_0) \right\} \\
& + (Z/k_0) \Pi_5(3Z/k_0) \left\{ \Pi_8(Z/k_0) - \Pi_8((Z + \alpha_0)/k_0) \right\} \\
& + \Pi_5(Z/k_0) \left\{ \Pi_9(3Z/k_0) - \Pi_9((3Z + \alpha_0)/k_0) \right\} \\
& + \Pi_6(3Z/k_0) \left\{ \Pi_8(Z/k_0) - \Pi_8((Z + \alpha_0)/k_0) \right\} \\
& + \Pi_8(Z/k_0) \left\{ \Pi_3(2Z/k_0) - \Pi_3((2Z + \alpha_0)/k_0) \right\} \\
& + \Pi_5(Z/k_0) \left\{ \Pi_7((2Z/k_0) - \Pi_7((2Z + \alpha_0)/k_0)) \right\} \\
& - \Pi_5(Z/k_0) \left\{ \Pi_9(2Z/k_0) - \Pi_9((2Z + \alpha_0)/k_0) \right\} \left. \right]
\end{aligned}$$

$$\begin{aligned}
B_{22} = \frac{8Z^3}{k_0^3} & \left[\frac{(k_0^2 + 4Z - Z^2)}{2k_0} \left\{ (\Pi_8(Z/k_0) - \Pi_8((Z+\alpha_0)/k_0))^2 \right\} \right. \\
& + (1-2Z) \left\{ (\Pi_8(Z/k_0) - \Pi_8((Z+\alpha_0)/k_0)) (\Pi_9(Z/k_0) - \Pi_9((Z+\alpha_0)/k_0)) \right\} \\
& + (2Z/k_0) \left\{ (\Pi_8(Z/k_0) - \Pi_8((Z+\alpha_0)/k_0)) (\Pi_8(3Z/k_0) - \Pi_8((3Z+\alpha_0)/k_0)) \right\} \\
& + 2 \left\{ (\Pi_8(Z/k_0) - \Pi_8((Z+\alpha_0)/k_0)) (\Pi_9(3Z/k_0) - \Pi_9((3Z+\alpha_0)/k_0)) \right\} \\
& + \Pi_8(Z/k_0) \left\{ \Pi_7(2Z/k_0) - \Pi_7((2Z+\alpha_0)/k_0) \right\} \\
& - \Pi_8((Z+\alpha_0)/k_0) \left\{ \Pi_7((2Z+\alpha_0)/k_0) - \Pi_7((2Z+2\alpha_0)/k_0) \right\} \\
& - \Pi_5(Z/k_0) \left\{ \Pi_3(2Z/k_0) - \Pi_3((2Z+\alpha_0)/k_0) \right\} \\
& \left. + \Pi_5((Z+\alpha_0)/k_0) \left\{ \Pi_3((2Z+\alpha_0)/k_0) - \Pi_3((2Z+2\alpha_0)/k_0) \right\} \right]
\end{aligned}$$

$$\begin{aligned}
B_{2n} = \frac{8Z^3}{k_0} & \left[\left\{ \frac{\Pi_8(Z/k_0) - \Pi_8((Z+\alpha_0)/k_0)}{k_0} \right\} \left\{ \frac{(k_0^2 + 4Z - Z^2)}{(Z+\beta_n)^3} \right. \right. \\
& + \frac{(1-Z)}{(Z+\beta_n)^2} + \frac{2Z}{(3Z+\alpha_0)^3} + \frac{1}{(3Z+\beta_n)^2} \left. \right\} \\
& + 2Z \left\{ \frac{\Pi_8(3Z/k_0) - \Pi_8(3Z+\alpha_0)/k_0}{k_0(Z+\beta_n)^3} \right\} - 2 \left\{ \frac{\Pi_9(Z/k_0) - \Pi_9((Z+\alpha_0)/k_0)}{(Z+\beta_n)^3} \right\} \\
& + 2 \left\{ \frac{\Pi_9(3Z/k_0) - \Pi_9(3Z+\alpha_0)/k_0}{(Z+\beta_n)^2} \right\} + \left\{ \frac{\Pi_8((2Z+\beta_n)/k_0) - \Pi_8((2Z+\beta_n+\alpha_0)/k_0)}{k_0(Z+\beta_n)^2} \right\} \\
& + 2(1-Z) \left\{ \frac{\Pi_9(Z/k_0) - \Pi_9((Z+\alpha_0)/k_0)}{(Z+\beta_n)^3} \right\} \\
& \left. + 2 \left\{ \frac{\Pi_9((2Z+\beta_n)/k_0) - \Pi_9((2Z+\beta_n+\alpha_0)/k_0)}{(Z+\beta_n)^3} \right\} \right]
\end{aligned}$$

$$\begin{aligned}
B_{n1} = & \frac{8Z^3}{k_0} \left[\frac{\Pi_5(Z/k_0)}{k_0} \left\{ \frac{(k_0^2 + 4Z - Z^2)}{(Z + \beta_n)^3} + \frac{(1-Z)}{k_0(Z + \beta_n)^2} + \frac{2Z}{k_0(3Z + \beta_n)^3} + \frac{1}{k_0(3Z + \beta_n)^2} \right\} \right. \\
& + \frac{2Z\Pi_5(3Z/k_0)}{k_0(Z + \beta_n)^3} + \frac{2\Pi_6(3Z/k_0)}{(Z + \beta_n)^3} + \frac{\Pi_8(Z/k_0)\Pi_3((2Z + \beta_n)/k_0)}{k_0^3} \\
& \left. + \frac{2(1-Z)\Pi_6(Z/k_0)}{(Z + \beta_n)^3} - \frac{\Pi_5(Z/k_0)}{k_0(Z + \beta_n)^2} + \frac{\Pi_5(Z/k_0)\Pi_8((2Z + \beta_n)/k_0)}{k_0^3} \right]
\end{aligned}$$

$$\begin{aligned}
B_{n2} = & \frac{8Z^3}{k_0} \left[\left(\frac{\Pi_8(Z/k_0) - \Pi_8((Z + \alpha_0)/k_0)}{k_0} \right) \left\{ \frac{(k_0^2 + 4Z - Z^2)}{(Z + \beta_n)^3} + \frac{(1-Z)}{(Z + \beta_n)^2} \right. \right. \\
& + \frac{2Z}{(3Z + \alpha_0)^3} + \left. \frac{1}{(3Z + \beta_n)^2} \right\} - \frac{\Pi_8(Z/k_0)}{k_0(Z + \beta_n)^2} + \frac{\Pi_8((Z + \alpha_0)/k_0)}{k_0(Z + \beta_n)^2} \\
& + 2(1-Z) \left\{ \frac{\Pi_9(Z/k_0) - \Pi_9((Z + \alpha_0)/k_0)}{(Z + \beta_n)^3} \right\} + \left\{ \frac{\Pi_8(Z/k_0)\Pi_8((2Z + \beta_n)/k_0)}{k_0^3} \right\} \\
& + 2Z \left\{ \frac{\Pi_8(3Z/k_0) - \Pi_8((3Z + \alpha_0)/k_0)}{k_0(Z + \beta_n)^3} \right\} + 2 \left\{ \frac{\Pi_9(3Z/k_0) - \Pi_9(3Z + \alpha_0)/k_0}{(Z + \beta_n)^2} \right\} \\
& - \left\{ \frac{\Pi_8((Z + \alpha_0)/k_0) \cdot \Pi_8((2Z + \beta_n + \alpha_0)/k_0)}{k_0^3} \right\} - \left\{ \frac{\Pi_5(Z/k_0) \cdot \Pi_5((2Z + \beta_n)/k_0)}{k_0^3} \right\} \\
& \left. + \left\{ \frac{\Pi_5((Z + \alpha_0)/k_0) \cdot \Pi_5((2Z + \beta_n + \alpha_0)/k_0)}{k_0^3} \right\} \right]
\end{aligned}$$

$$\begin{aligned}
B_{nm} = 8Z^3 & \left[\frac{2(k_0^2 + 4Z - Z^2)}{(Z + \beta_n)^3 (Z + \beta_m)^3} + \frac{2(1 - Z)}{(Z + \beta_n)^3 (Z + \beta_m)^2} \right. \\
& + \frac{2(1 - Z)}{(Z + \beta_n)^2 (Z + \beta_m)^3} + \frac{4Z}{(Z + \beta_n)^3 (3Z + \beta_m)^3} \\
& + \frac{4Z}{(3Z + \beta_n)^3 (Z + \beta_m)^3} + \frac{2}{(Z + \beta_n)^3 (3Z + \beta_m)^2} \\
& + \frac{2}{(3Z + \beta_n)^2 (Z + \beta_m)^3} + \frac{2}{(Z + \beta_n)^2 (Z + \beta_m)^2} \\
& \left. - \frac{2}{(Z + \beta_m)^2 (2Z + \beta_n + \beta_m)^3} - \frac{2}{(Z + \beta_m)^3 (2Z + \beta_n + \beta_m)^2} \right]
\end{aligned}$$

APPENDIX C The Definite Integrals

In this appendix we list the definite integrals used to calculate the **A** and **B** matrix elements. The source used in the evaluation of the integrals is Gradshteyn and Ryzhik (Ref. 24).

$$\Pi_1(\gamma) = \frac{2}{\gamma(\gamma^2+4)} \quad \gamma > 0$$

$$\Pi_2(\gamma) = \frac{1}{4} \ln \left(\frac{\gamma^2+4}{\gamma^2} \right) \quad \gamma > 0$$

$$\Pi_3(\gamma) = \frac{1}{(\gamma^2+4)} \quad \gamma > 0$$

$$\Pi_4(\gamma) = \frac{1}{2} \tan^{-1} \left(\frac{2}{\gamma} \right) \quad \gamma > 0$$

$$\Pi_5(\gamma) = \frac{2\gamma}{(\gamma^2+1)^2} \quad \gamma > 0$$

$$\Pi_6(\gamma) = \frac{1}{(\gamma^2+1)} \quad \gamma > 0$$

$$\Pi_7(\gamma) = \frac{1}{\gamma} \left(1 - \frac{2}{(\gamma^2+4)} \right) \quad \gamma > 0$$

$$\Pi_8(\gamma) = \frac{\gamma^2-1}{(\gamma^2+1)^2} \quad \gamma > 0$$

$$\Pi_9(\gamma) = \frac{\gamma}{(\gamma^2+1)} \quad \gamma > 0$$

VITA

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the collisional cross-section for elastic scattering as a function of incident electron energy.

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